Spectroscopy in high- temperature industrial processes on Earth

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Spectroscopy in high- temperature industrial processes on Earth

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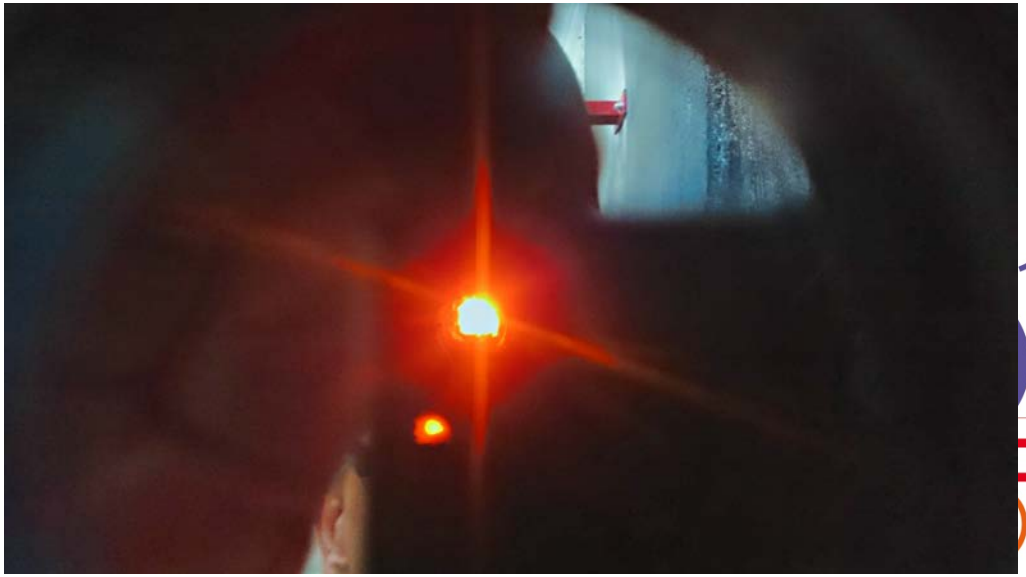
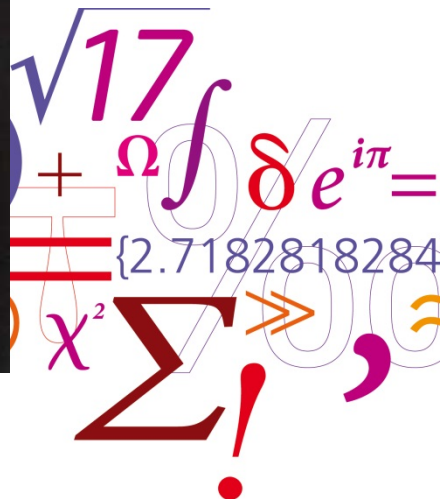
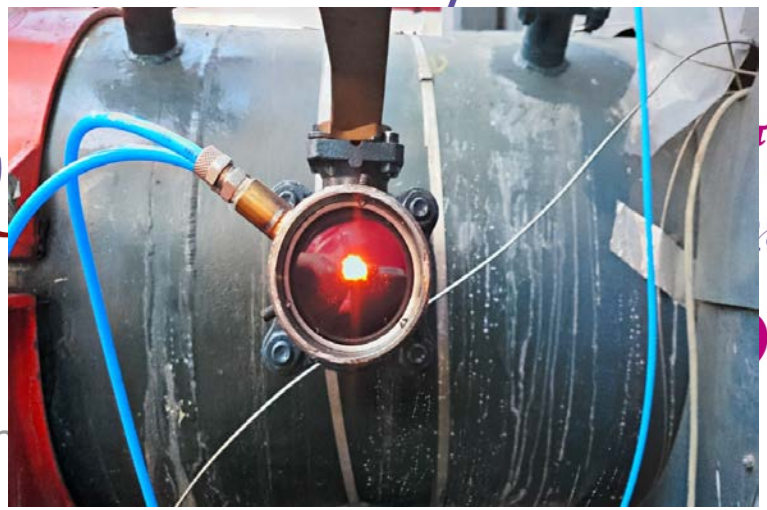




DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

Outline

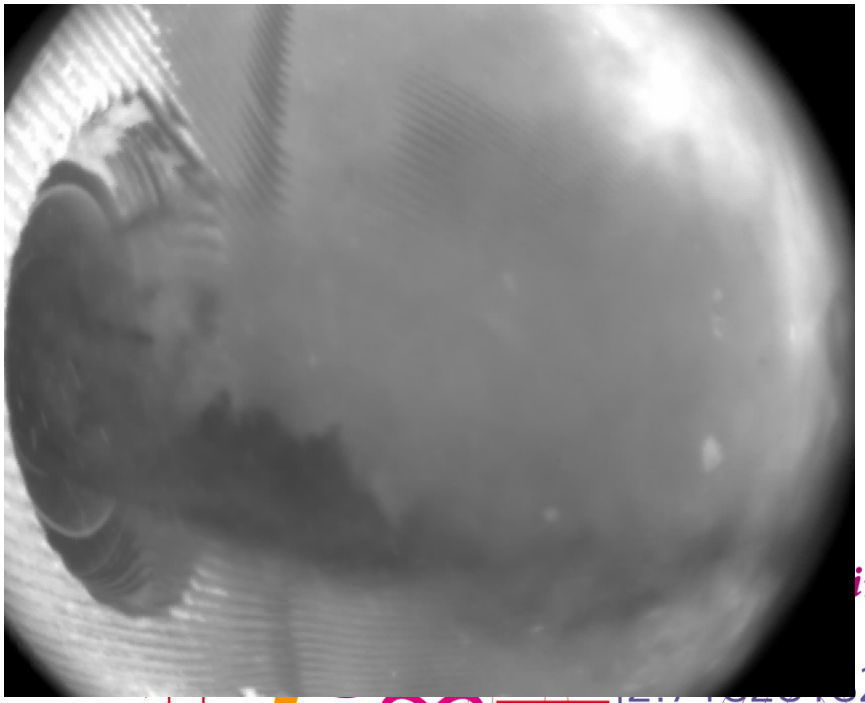
- **Background**
- **Large scale measurements**
- **Example/Case 1: NH3**
- **Example/Case 2: SO2/SO3**
- **Example/Case 3/UV: C6H6O and C10H8**
- **Conclusions**



Needs | # Large Scale Measurements

- Boilers,
- Flames (oil, gas, bio-masses),
- Engines (ships, jets),
- Field campaigns (explosions)

VIS image grade flame (waste)



IR image wood dust flame (video fuel mixing)

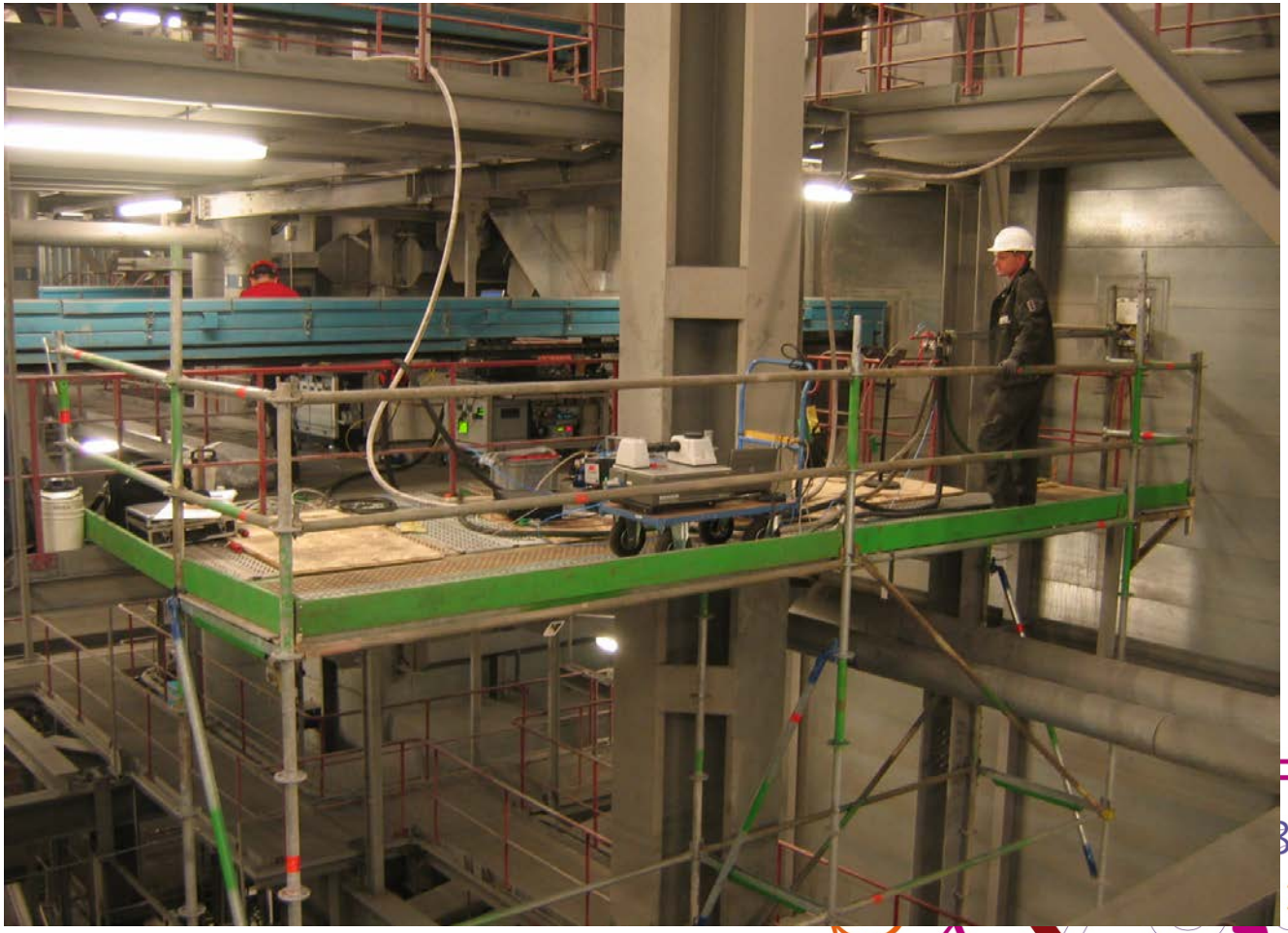
Large Scale Measurements

Complexity:

- get results first
- trustful system
- 1500C is not uncommon

Expensive:

- access possibilities
- man power
- time



Campaign at Blok 7 Fynsværket (Denmark)

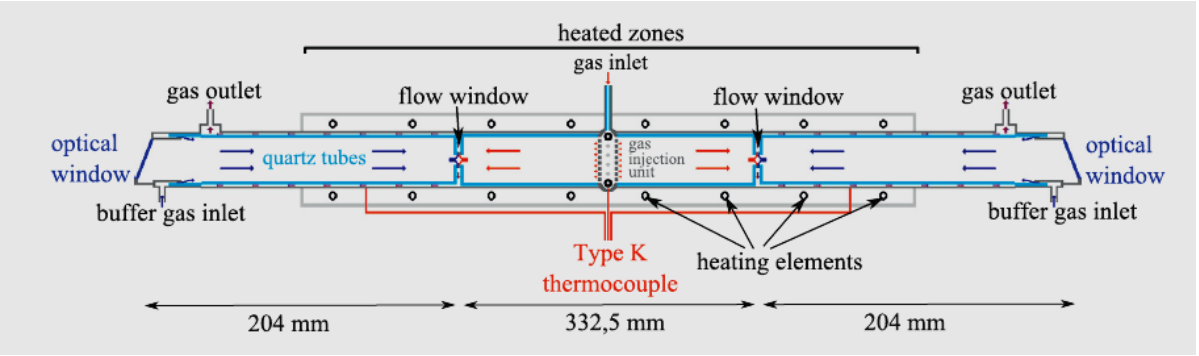
Large Scale Measurements

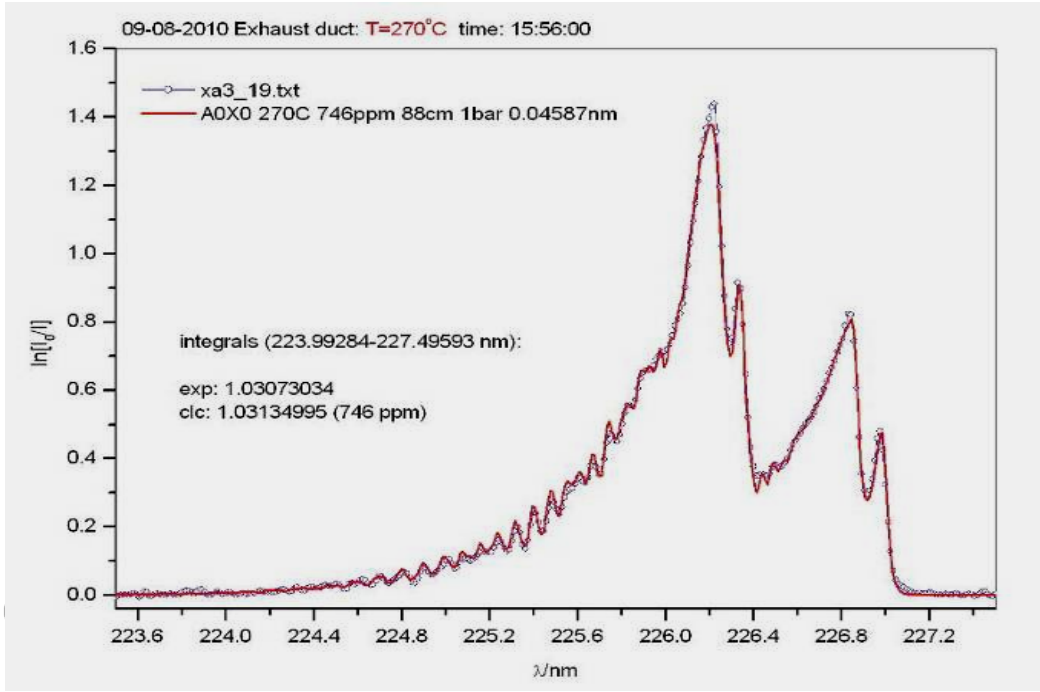
Data analysis:

- on-line
- at home

Source of reference data:

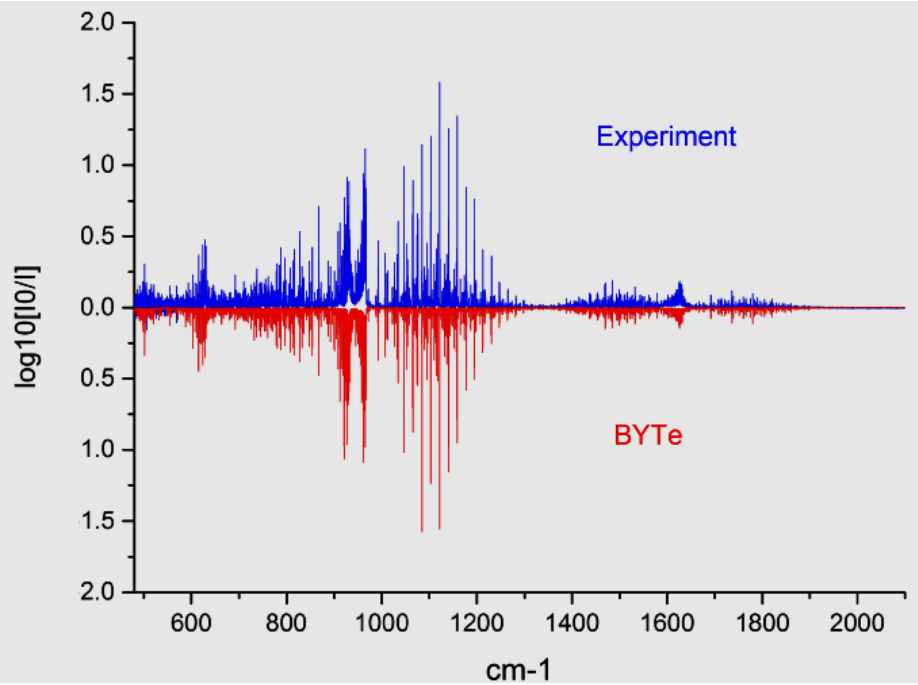
- measurements in a cell with pre-mixed gases
- **databases (IR/UV)**





NO measurements in exhaust duct of a large ship engine

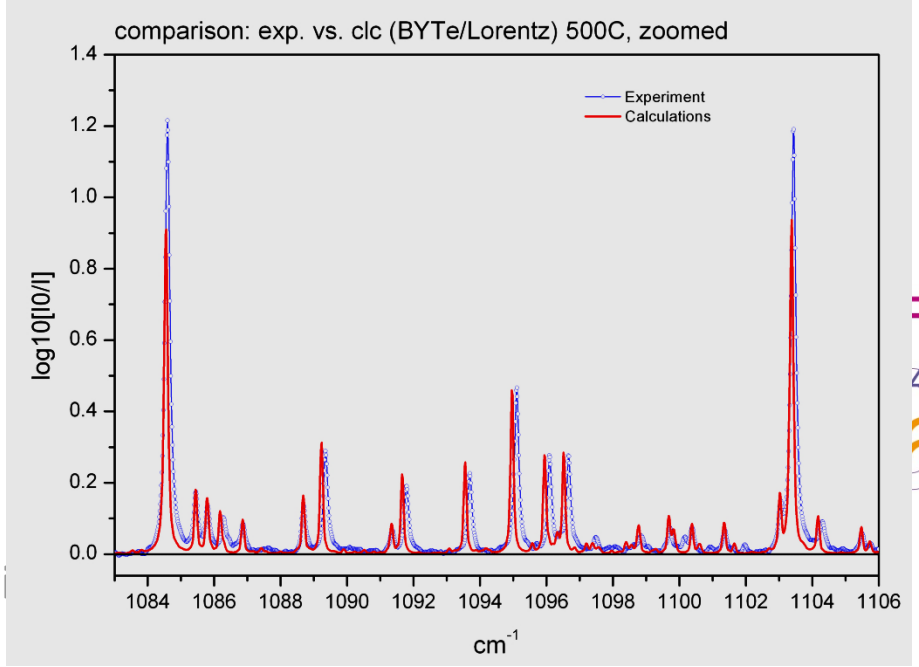
Example 1 | NH3: experiment (500C, 0.09cm-1) vs calculations (BYTe)



Can we use BYTe at 500C for practical apps?

- in general a good agreement
- some difficulties with strong line intensities
- some frequency shifts in line positions

More work to do at even higher T (>500C)

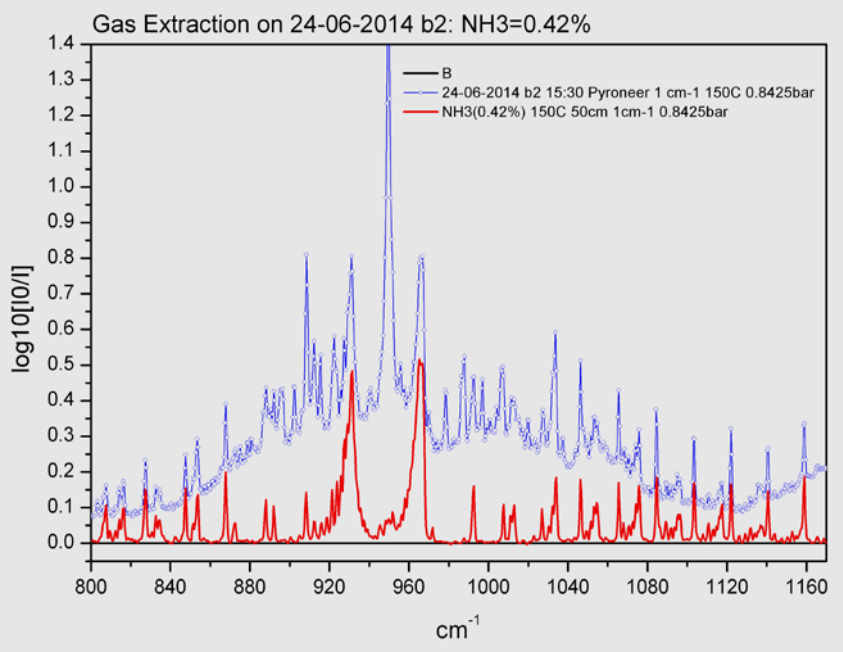


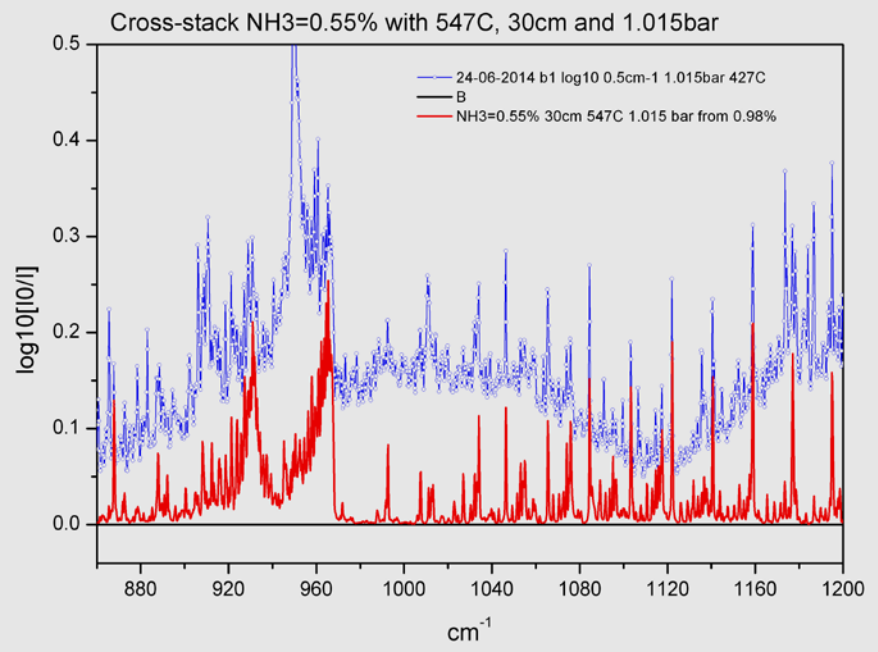
More details:

Emma J. Barton et al
"High-resolution absorption measurements of NH3 at high temperatures: 500 - 2100 cm-1"
(submitted to JQSRT)

In Situ measurements on **Pyroneer (6MW) gasifier**

NH3: Q: Why to do measurements? A: NH3 contributes to NOx formation





Gas extraction (150C):

20-06-2014 (17:00-19:30) : **NH3=(0.4 ± 0.02)%,** H2O=(35 ± 0.6)%, CO2=(14 ± 0.45)%, CO=(10 ± 0.21)%

24-06-2014 (15:00-17:00): **NH3=(0.42 ± 0.02)%,** H2O=(36 ± 0.6)%, CO2=(13.5 ± 0.45)%, CO=(10.3 ± 0.21)%

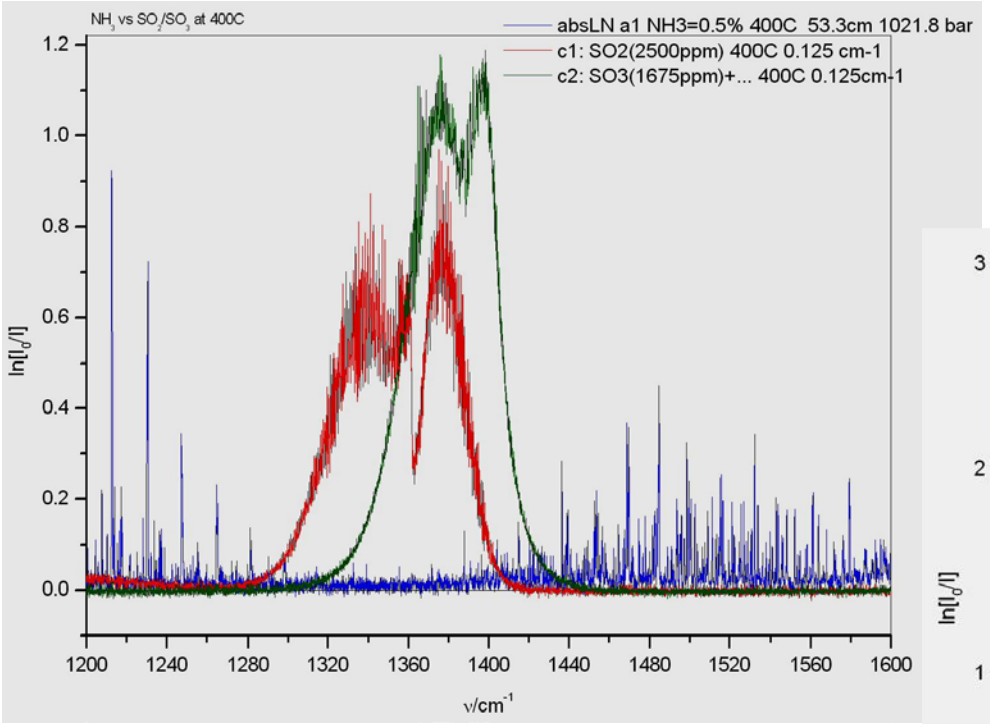
In situ (547C):

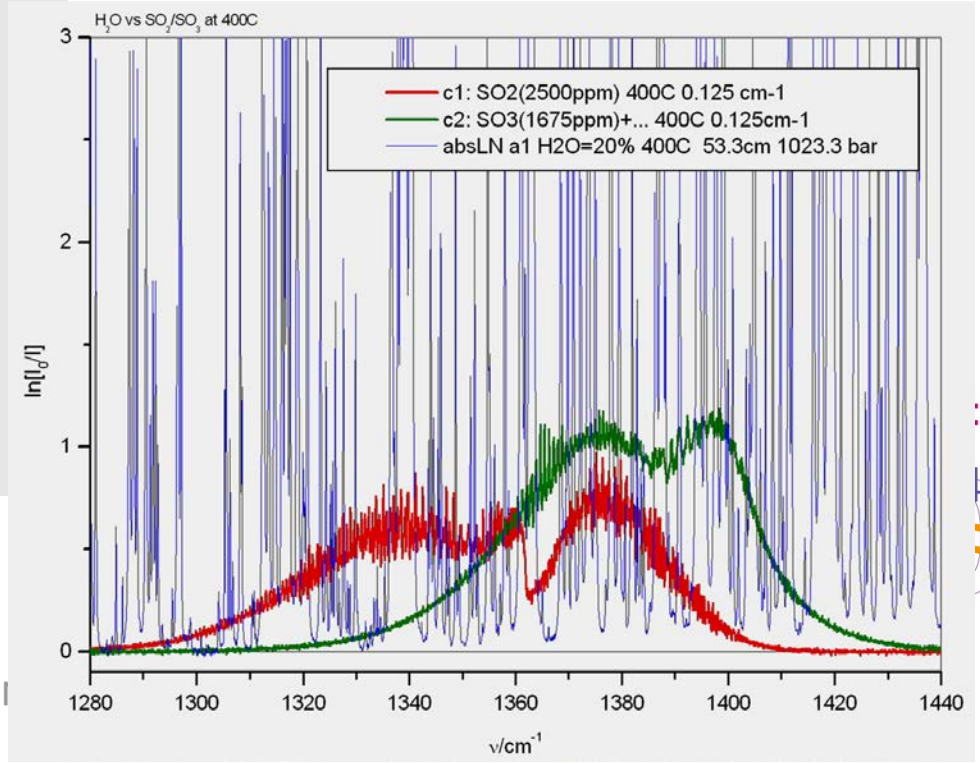
24-06-2014 (20:00-21:00): **NH3=(0.55 ± 0.05)%,** H2O=(36 ± 1)%

Application case 2 | # SO2/SO3/NH3 in a hot flue gas

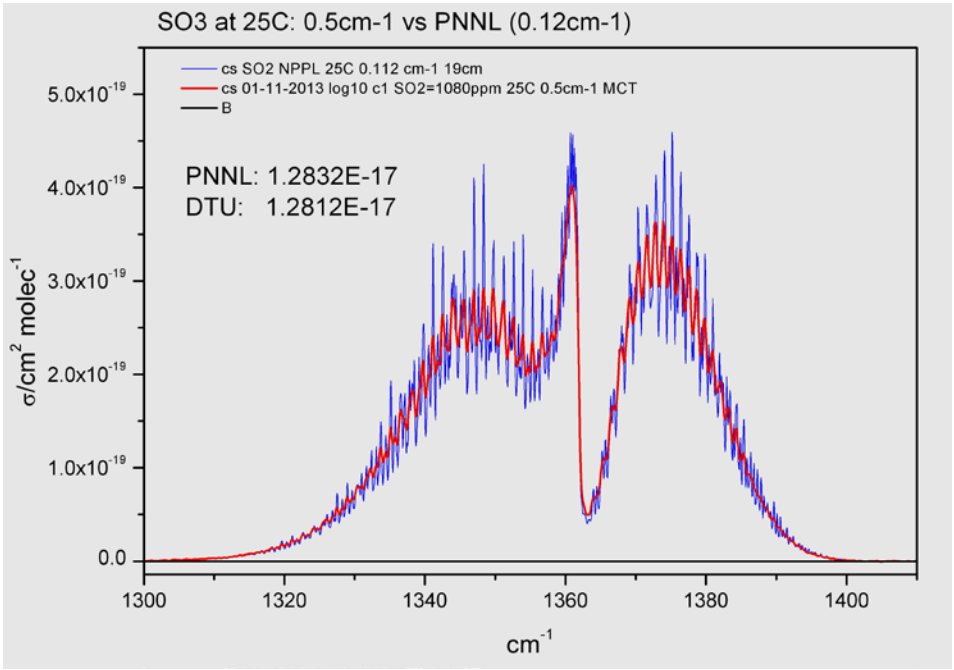
SO2/SO3/NH3: **Q: Why to do measurements?**

A: NOx reduction at SCR/NSCR units, NH3 slip/costs, corrosion/fouling

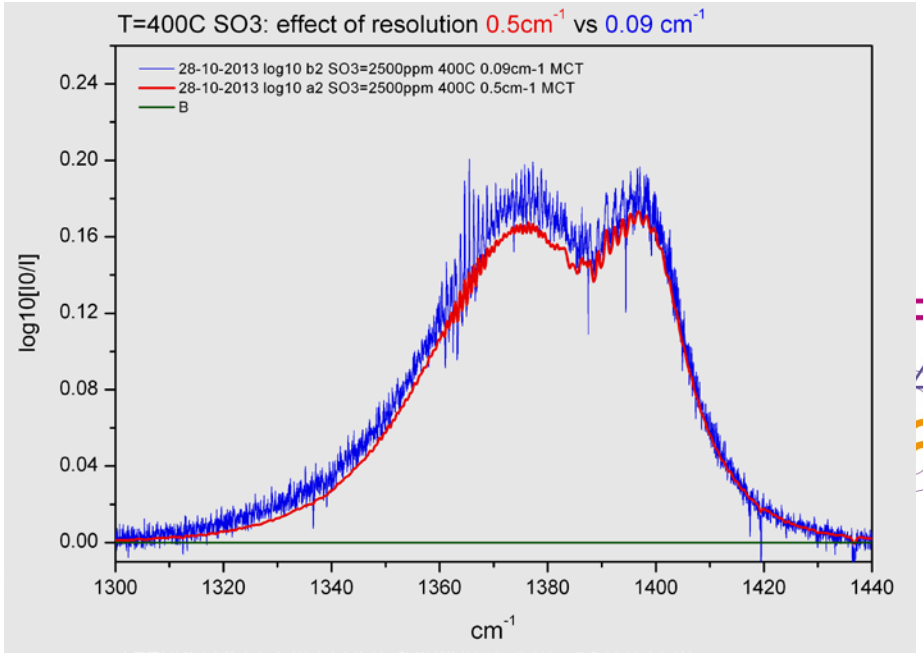




Example 2 | # SO3: measurements at 25C and 400C



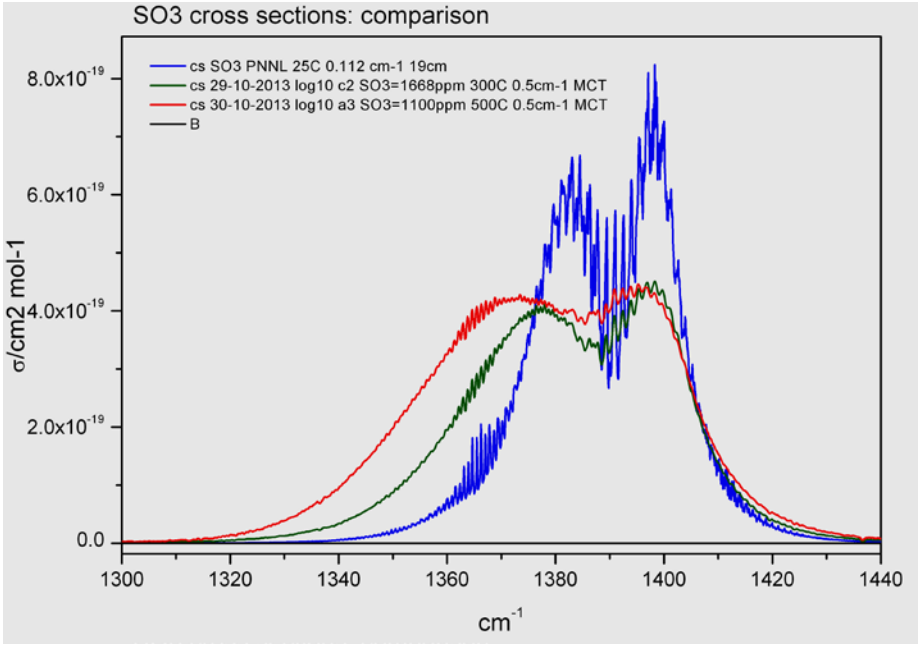
- Simple to generate, but difficult to measure/quantify
- No databases (SO2/SO3) are available at T>100C



Good news:

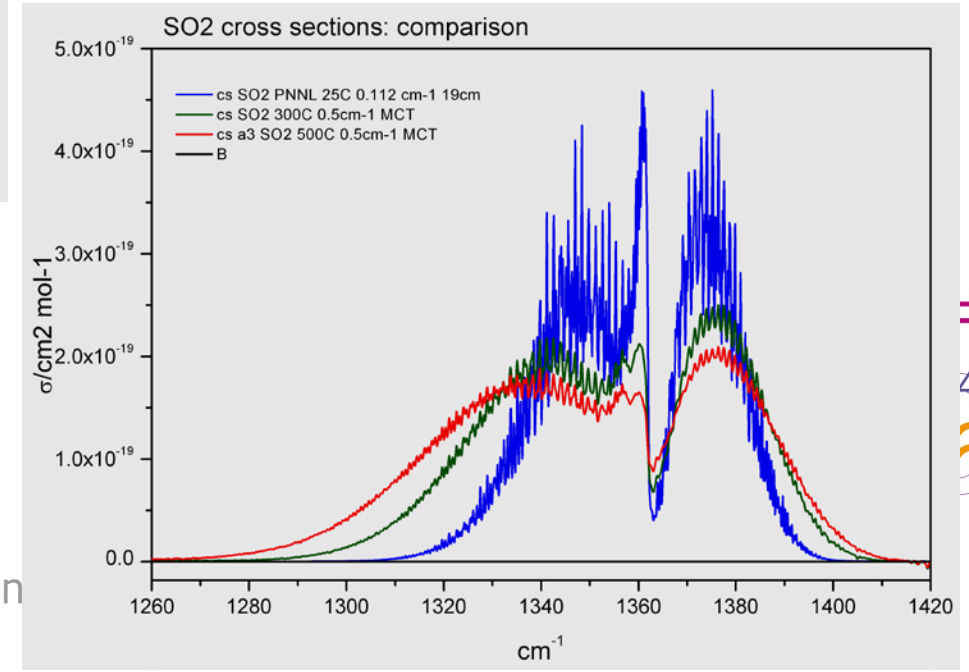
- Excellent agreement with PNNL data at 25C
- No need to use high-resolution at high T

Example 2 | SO2/SO3 cross sections (0.5cm-1)



PhD (Dan Underwood) with UCL:

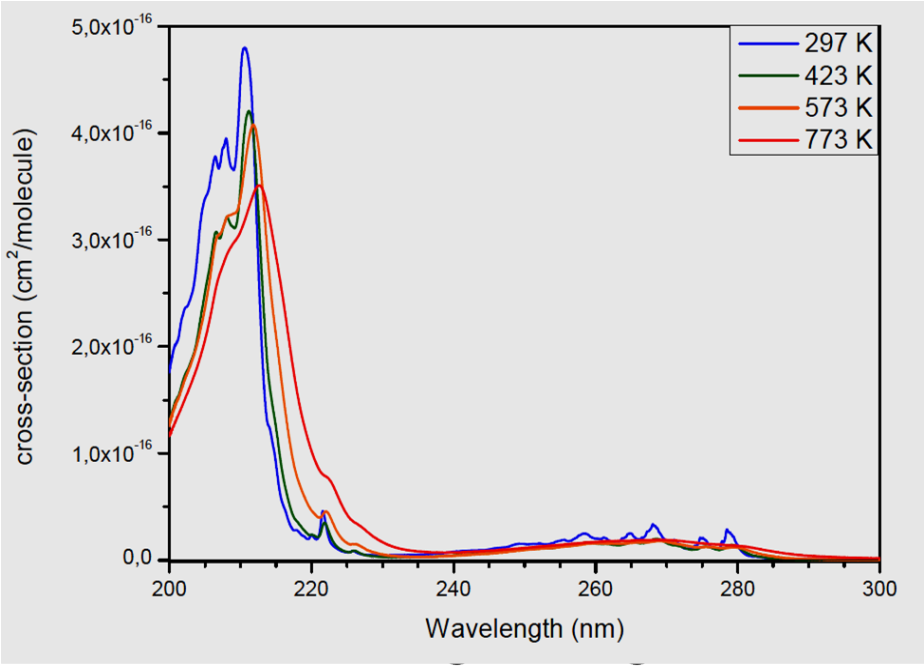
- SO_2 and SO_3 line lists
- ready by the end 2015
- **2nd Power plant measurement campaign, fall 2015**



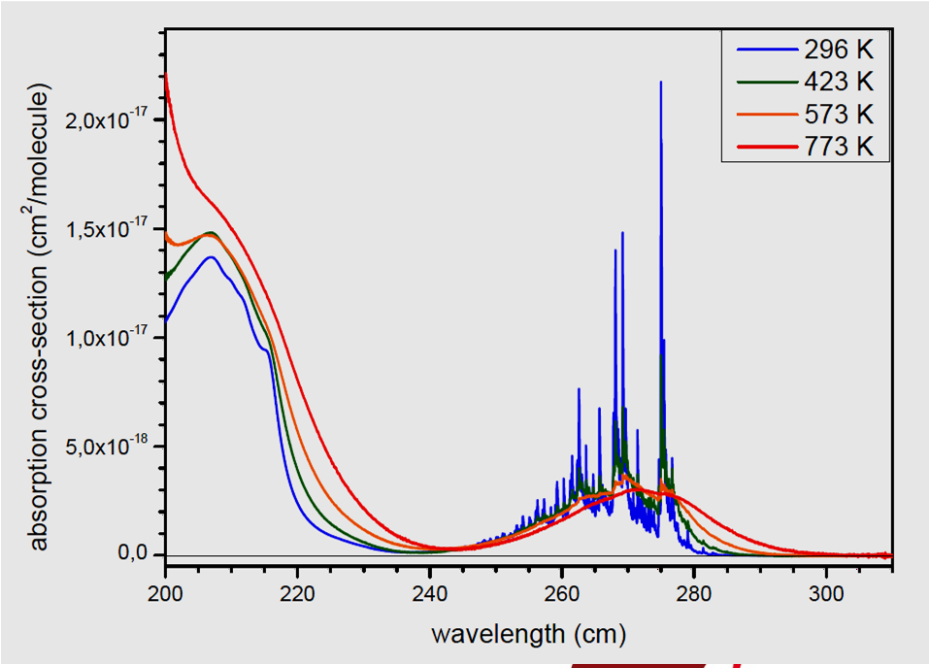
Phenol/Naphthalene UV absorption cross-sections temperature effects

- Not too many reference data available even at low T (about 23C)
- An excellent agreement with published data at low T
- Significant changes in the fine structure of the cross-section spectra with T

Naphthalene abs cross-sections: from 23C to 500C



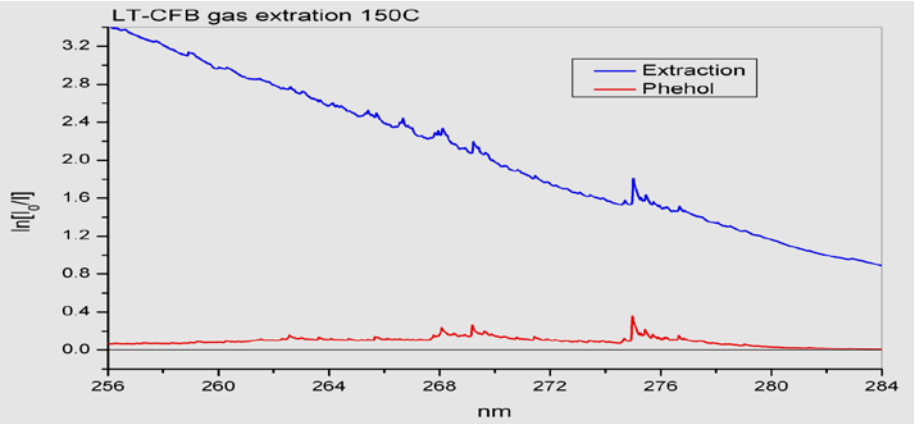
Phenol abs cross-sections: from 23C to 500C



Application case 3/UV | In Situ measurements **on LT-CFB (100kW) gasifier**

Phenol/Naphthalene: Q: Why to do measurements?

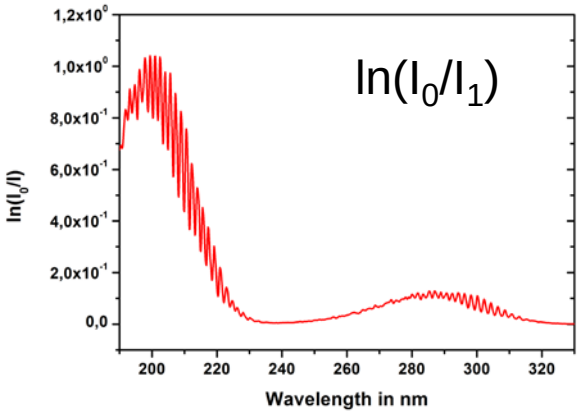
A: Phenol/Naphthalene – major trace gases from PAH's in low temperature gasification

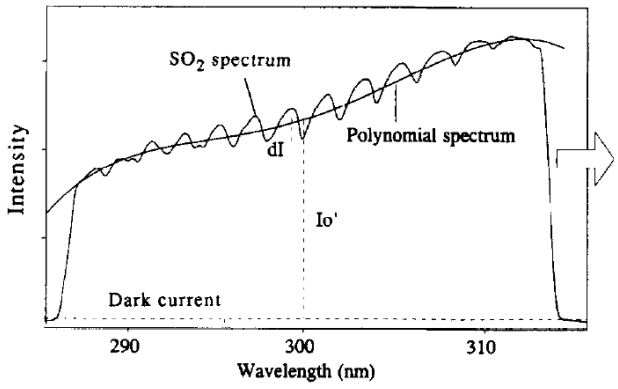


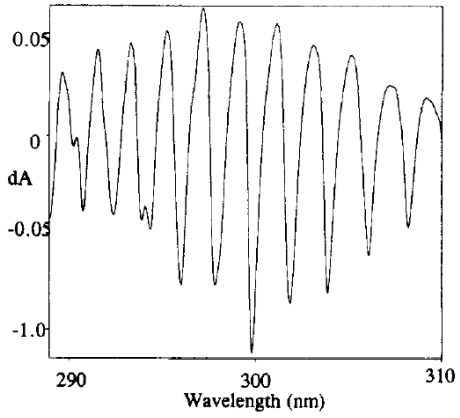
Few new challenges:

- Very strong UV light attenuation
- Very broad continuum-like abs structures
- Very small L for in situ measurements

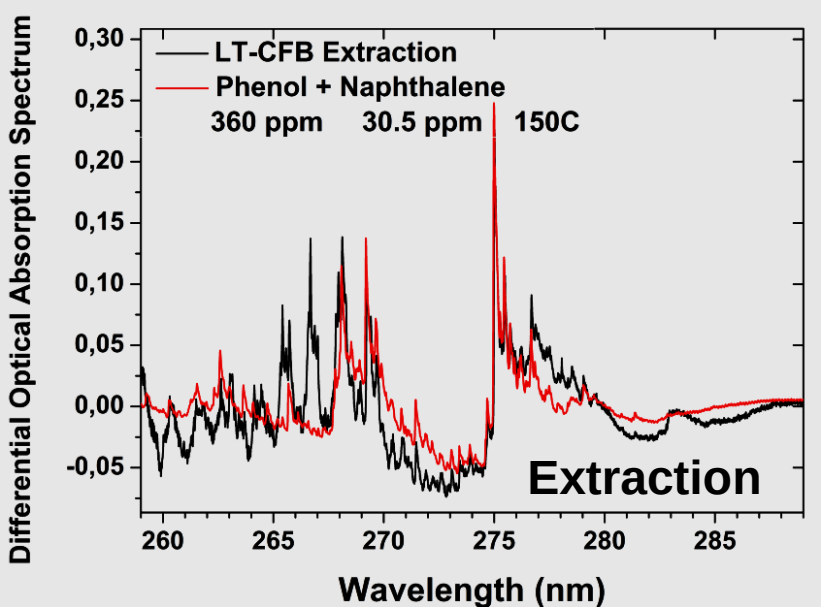
DOAS approach: SO2 UV absorption as an example

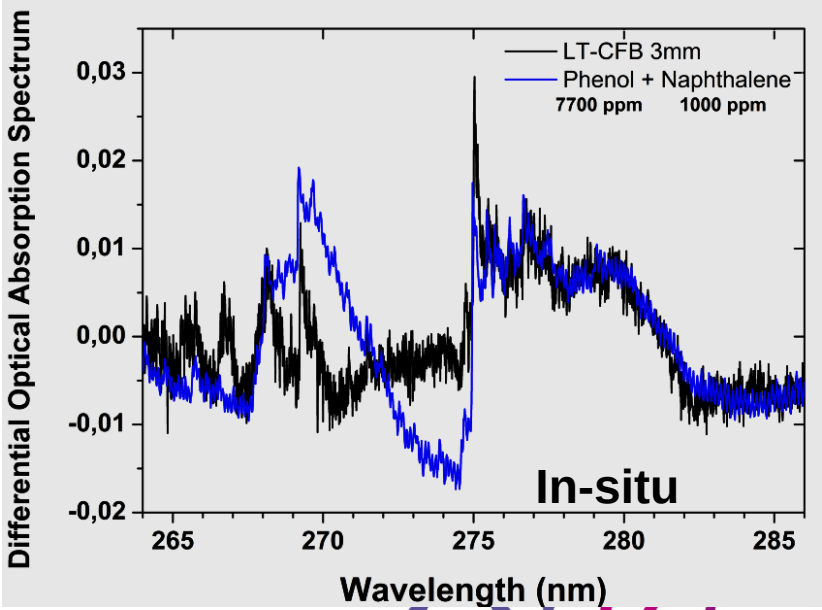






Comparison of the measurements





Method	Time	Temperature	Phenol	Naphthalene
GC-MS	30 min	15˚C	215 ppm	16 ppm
Extraction	3 min	150˚C	360 ppm	31 ppm
In-situ	3 min	306˚C	7700 ppm	1000 ppm

In general

- You can find a lot inspirations for the work on the Earth
- Different research areas can have the same origin
- Scientists can make industry guys happy

In particular:

- Excellent experimental tools are available for (VUV) UV-FIR optical measurements
- Temperature range can be also negative (e.g. gases at low T)
- New data/lines for NH3/SO2/SO3
- New data for phenol/naphthalene
- Try always In Situ and avoid any Ex Situ (extraction) measurements

Future

- Inspiration comes from industry (small, middle large, …)
- Possible spin offs: innovation (patents)
- New **gas components: CH3Cl, KCl etc. (together with UCL)**
- Combine several methods to obtain **multi-parameters**
- **… ?**
- Contact: Alexander Fateev
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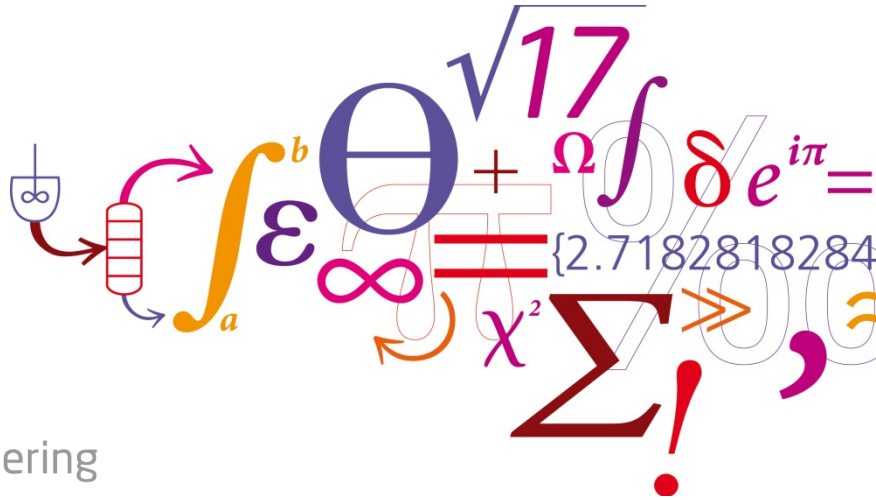

Acknowledgements

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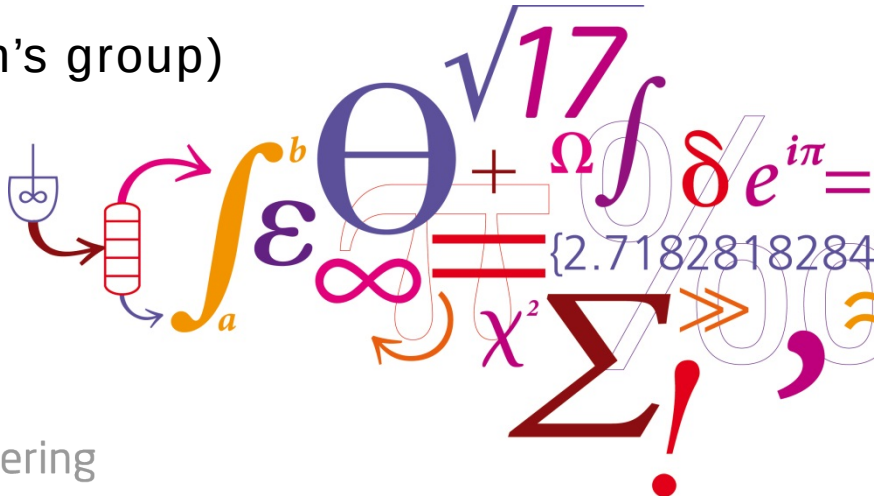
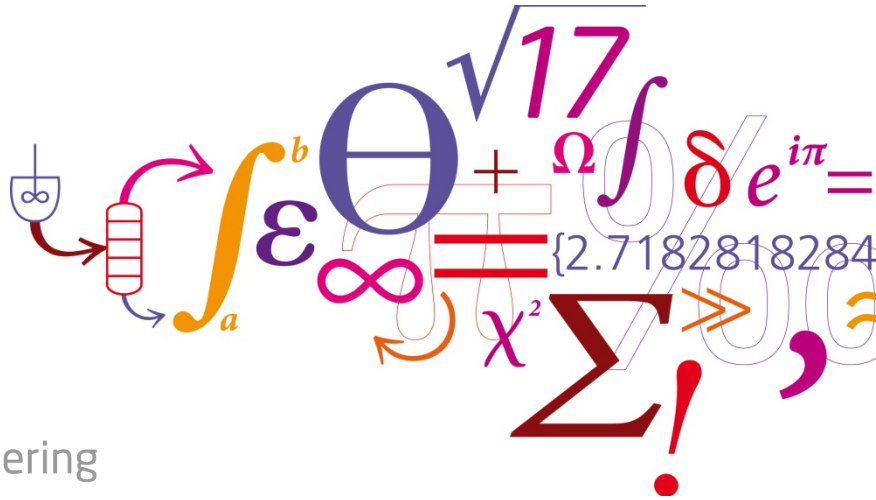
- To DONG Energy and Vattenfall
- To UCL (Prof. Jonathan Tennyson's group)



Thank you for your attention



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